Thermodynamic potentials from shifted boundary conditions: the scalar-field theory case

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Abstract

In a thermal field theory, the cumulants of the momentum distribution can be extracted from the dependence of the Euclidean path integral on a shift in the fields built into the temporal boundary condition. When combined with the Ward identities associated with the invariance of the theory under the Poincaré group, thermodynamic potentials such as the entropy or the pressure can be directly inferred from the response of the system to the shift. Crucially the argument holds, up to harmless finite-size and discretization effects, even if translational and rotational invariance are broken to a discrete subgroup of finite shifts and rotations such as in a lattice box. The formulas are thus applicable at finite lattice spacing and volume provided the derivatives are replaced by their discrete counterpart, and no additive or multiplicative ultraviolet-divergent renormalizations are needed to take the continuum limit. In this paper we present a complete derivation of the relevant formulas in the scalar field theory, where several technical complications are avoided with respect to gauge theories. As a by-product we obtain a recursion relation among the cumulants of the momentum distribution, and formulæ for finite-volume corrections to several well-known thermodynamic identities.

1 Introduction

Thermal field theory is the theoretical tool for computing properties of matter at high temperatures and densities from first principles [1, 2]. It allows one, for instance, to determine the equation of state of Quantum Chromodynamics, which in turn is an essential ingredient to understand the properties of matter created in heavy ion collisions, and to model the behavior of hot matter in the early universe (for recent reviews see Ref. [3, 4]). Obtaining first-principles predictions from a thermal field theory is often challenging since it describes an infinite number of degrees of freedom subject to both quantum and thermal fluctuations. Even though there are several established methods to compute the thermal properties of field theories [5–8], new theoretical concepts and more efficient computational techniques are still needed in many contexts particularly when weak-coupling methods are inapplicable.

In a recent Letter we related the generating function of the cumulants of the total momentum distribution to a path integral with properly chosen shifted boundary conditions in the compact direction normalized to the ordinary thermal one [9]. By exploiting the Ward Identities (WIs) associated with the space-time invariances of the continuum theory, the cumulants can be related in a simple manner to thermodynamic potentials. In a relativistic theory at zero chemical potential, for instance, the variance of the momentum probability distribution measures the entropy of the system. Thanks to a recursion relation among the cumulants, the kurtosis is related to the specific heat. These results suggested a new way to determine the equation of state of a thermal field theory [9].

The aim of this paper is to present a complete and self-contained derivation of the formulas introduced in Ref. [9] for the scalar field theory, where several technical complications in their derivation are avoided with respect to gauge theories [10]. A crucial rôle is played by the symmetry-constrained path integrals [11,12] and by the continuum WIs associated with the relativistic invariance of the theory. The latter allow us to derive the recursive relation among the cumulants, to generalize well-known thermodynamic relations to finite-volume systems, and to exclude additive or multiplicative ultraviolet-divergent renormalizations of the cumulants. The formulas are applicable, up to harmless finite-size and discretization effects, at finite volume and lattice spacing, where ratios of path integrals can be determined by *ab initio* Monte Carlo computations [9]. As a result the entropy density, the pressure and the specific heat of a thermal field theory can be obtained by studying the response of the system to the bare shift parameter.

After a section on the basic properties of the scalar theory, the symmetry-constrained path integral and its relation with the cumulant generator is introduced in section 3. The relevant WIs are derived in sections 4 to 6, and the main results and conclusions of the paper are reported in section 7. Several technical details are given in the four appendices.

2 Preliminaries and basic notation

We are interested in the thermal scalar theory defined via the Euclidean path integral formalism in an infinite volume as well as in a finite box of volume[1] $V = L^3$ with the field ϕ satisfying periodic boundary conditions. The time extent is set to $L_0 = 1/T$, where T is the temperature of the system. Some basic definitions and WIs, associated with the invariance of the continuum theory under the Poincaré group, are reviewed in this section. Other properties of the theory, not directly relevant for the subject of this paper, can be found in various textbooks, see for instance Refs [13, 14].

The partition function of the theory is defined as usual as

$$Z = \int D\phi \, e^{-S} \, , \tag{2.1}$$

where the action $S = \int d^4x \, \mathcal{L}$ is defined by the Lagrangian density

$$\mathcal{L} = \frac{1}{2} (\partial_\mu \phi)(\partial_\mu \phi) + V(\phi) \, , \qquad V(\phi) = \frac{1}{2} m^2 \phi^2 + \frac{\lambda}{4!} \phi^4 \, . \tag{2.2}$$

The equations of motion are given by

$$\left\langle \left\{ \frac{\partial V}{\partial \phi} - \Box \phi \right\}(x) \, O_1 \dots O_n \right\rangle = \sum_{i=1}^{n} \langle \, O_1 \dots O_i' \dots O_n \, \rangle \, , \tag{2.3}$$

where O_i is a generic local field[2] inserted at the point x^i, and O_i' is its variation with respect to the fundamental field and its derivative at the coordinate value x.

2.1 Translational invariance

The theory is invariant under space-time translations, i.e. under the direct product of four continuum Abelian groups of global transformations

$$x'_\mu = x_\mu - \varepsilon_\mu \, , \qquad \phi'(x'_\mu) = \phi(x_\mu) \, . \tag{2.4}$$

The associated WIs can be derived in the usual way by promoting the symmetry to a local one, i.e. $\varepsilon_\mu \to \varepsilon_\mu(x)$, and studying the variation of the functional integral under the local transformations

$$\delta\phi(x) = \varepsilon_\mu(x) \, \partial_\mu \phi(x) \, , \qquad \delta\{\partial_\nu \phi(x)\} = \partial_\nu \{\varepsilon_\mu(x) \partial_\mu \phi(x)\} \, . \tag{2.5}$$

By considering different functions $\varepsilon_\mu(z)$ and properly chosen fields O_i, many interesting non-trivial relations can be derived. For $\varepsilon_\nu(z) = \epsilon_\nu \delta^{(4)}(z - x)$ one obtains

$$\epsilon_\nu \, \langle \partial_\mu T_{\mu\nu}(x) \, O_1 \dots O_n \rangle = - \sum_{i=1}^{n} \, \langle O_1 \dots \delta^x_\epsilon O_i \dots O_n \rangle \, , \tag{2.6}$$

[1] Throughout the paper the linear dimension in the spatial direction k will be indicated by L_k.

[2] Sometimes the argument x^i is shown explicitly to clarify the meaning of some formulas. Summation over repeated indices is understood unless explicitly specified. No summation over k is understood in sections 4 to 6, and everywhere for the field T_{kk}.

where $\delta_\epsilon^x O_i$ is the variation of the field O_i under the transformation (2.5), and the field

$$T_{\mu\nu} = (\partial_\mu \phi)(\partial_\nu \phi) - \delta_{\mu\nu} \mathcal{L} \tag{2.7}$$

is the energy-momentum tensor of the theory symmetric under the exchange $\mu \leftrightarrow \nu$. The WIs (2.6), and therefore the consequences discussed in the following, applies to connected correlation functions as well. When all operators O_i are localized far away from x, the classical conservation identities

$$\langle \partial_\mu T_{\mu\nu}(x)\, O_1 \ldots O_n \rangle = 0 \tag{2.8}$$

are recovered. If we integrate Eq. (2.6) over a bounded region R which contains in its interior the points $x^1, \ldots, x^m$ while the fields $O_{m+1} \ldots O_n$ are localized outside, the Gauss theorem leads to

$$\epsilon_\nu \int_{\partial R} d\sigma_\mu(x)\, \langle T_{\mu\nu}(x) O_1 \ldots O_n \rangle = - \sum_{i=1}^{m} \langle O_1 \ldots \delta_\epsilon O_i \ldots O_n \rangle \;, \tag{2.9}$$

where $\delta_\epsilon O_i$ is the variation of the field O_i under the *global* transformation associated with ϵ_ν, and the integration measure $d\sigma_\mu(x)$ points along the outward normal to the surface ∂R. In this case, the very same WIs could have been obtained by considering directly the limit where $\varepsilon_\nu(x)$ goes to a constant in R, and it is null outside.

The discussion above applies also to the theory defined in a finite box with periodic boundary conditions, provided the δ-function is replaced by its periodic generalization $\delta^{(\mathrm{p})}$. In the following we will use the same notation for both of them since the precise meaning will be clear from the context.

2.2 Time evolution of operators

From the WIs in Eq. (2.9) we can derive the time-evolution of a generic field. If we choose $\epsilon_\nu = \delta_{\nu 0} \epsilon_0$, and we integrate over a thick time-slice R with the field O_1 being an arbitrary functional of ϕ and $\partial_\mu \phi$ inserted into it while the operators $O_2 \ldots O_n$ are localized outside, then

$$\delta O_1(x) = \epsilon_0\, \partial_0 O_1(x) \tag{2.10}$$

and therefore

$$\partial_0 \, \langle O_1(x^1)\, O_2 \ldots O_n \rangle = - \int_{\partial R} d\sigma_0(x)\, \langle T_{00}(x)\, O_1(x^1)\, O_2 \ldots O_n \;\rangle \;. \tag{2.11}$$

This is the Euclidean version of the time-evolution of the generic field $O_1(x^1)$. The field

$$\overline{T}_{00}(x_0) = \int d^3\mathbf{x}\, T_{00}(x) \tag{2.12}$$

is therefore (minus) the Hamiltonian of the system, and we can write

$$\langle \overline{T}_{00} \rangle = \frac{\partial}{\partial L_0} \ln Z \;, \tag{2.13}$$

or more generally

$$\langle \overline{T}_{00}(L_0)\, O\rangle_c = \frac{\partial}{\partial L_0}\,\langle O\rangle\ , \tag{2.14}$$

where O is a generic operator which does not depend explicitly on the time coordinate and it is at a physical distance from the time-slice L_0.

2.3 Translational invariance of correlators

If all fields $O_1,\ldots,O_n$ are inside the integration region R, then the transformation (2.5) implies

$$\delta O_i(x) = \epsilon_\mu\, \partial_\mu O_i(x) \tag{2.15}$$

for arbitrary functionals of ϕ and $\partial_\mu\phi$. In the limit where the bounded region R goes to infinity or, for instance, in a finite volume with periodic boundary conditions, the l.h.s. of Eq. (2.9) can be neglected[3]. Correlation functions enjoy translational invariance, i.e. they satisfy

$$\sum_{i=1}^{n} \partial_\mu^{x^i}\ \langle O_1(x^1)\ldots O_i(x^i)\ldots O_n(x^n)\rangle = 0\ . \tag{2.16}$$

As an example of transformation of a composite field, it is interesting to study the variation of the energy-momentum tensor under local transformations. If we rewrite the tensor (2.7) as

$$T_{\mu\nu} = \frac{1}{2}\, R_{\mu\nu\alpha\beta}\,(\partial_\alpha\phi)(\partial_\beta\phi) - \delta_{\mu\nu}V(\phi)\ , \qquad R_{\mu\nu\alpha\beta} = \delta_{\mu\alpha}\delta_{\nu\beta} + \delta_{\mu\beta}\delta_{\nu\alpha} - \delta_{\mu\nu}\delta_{\alpha\beta}\ , \tag{2.17}$$

its variation under a local space-time translation (2.5) can be written as

$$\delta T_{\mu\nu}(x) = \varepsilon_\rho(x)\,\partial_\rho T_{\mu\nu}(x) + R_{\mu\nu\alpha\beta}\,\{T_{\rho\beta}(x) + \delta_{\rho\beta}\mathcal{L}(x)\}\,\partial_\alpha\varepsilon_\rho(x)\ , \tag{2.18}$$

and Eq. (2.15) is satisfied if $\varepsilon_\rho(x)$ is constant.

2.4 Invariance under 4-dimensional rotations

In the Euclidean the invariance under the homogeneous Lorentz group is replaced by the symmetry under $SO(4)$ rotations. An infinitesimal transformation reads

$$x'_\alpha = x_\alpha + \omega_{\alpha\beta}\, x_\beta \tag{2.19}$$

with $\omega_{\alpha\beta} = -\omega_{\beta\alpha}$ and, as in the previous section, we can derive the associated WIs by studying the variation of the functional integral under an infinitesimal local transformation. The latter can be written as

$$x'_\alpha = x_\alpha - \varepsilon_\alpha(x)\ , \qquad \varepsilon_\alpha(x) = -\omega_{\alpha\beta}(x)\, x_\beta\ , \tag{2.20}$$

[3] In WIs associated to space-time translational invariance no boundary terms of this type are expected to contribute at infinity in the quantum theory, at variance of what happen in those associated with spontaneously broken symmetries.

and the fields transform accordingly to Eq. (2.5). If we choose $\omega_{\alpha\beta}(x) = w_{\alpha\beta}\delta^{(4)}(z-x)$, we obtain

$$w_{\alpha\beta}\,\langle \partial_\mu K_{\mu;\alpha\beta}(x)\,O_1\dots O_n\rangle = -2\sum_{i=1}^{n}\,\langle O_1\dots\delta^x_w O_i\dots O_n\rangle\ , \tag{2.21}$$

where

$$K_{\mu;\alpha\beta} = x_\alpha T_{\mu\beta} - x_\beta T_{\mu\alpha} \tag{2.22}$$

is an antisymmetric tensor for $\alpha \leftrightarrow \beta$. The WIs (2.21) are just combinations of those in Eqs. (2.6) since, thanks to the symmetry of $T_{\mu\nu}$, $\partial_\mu K_{\mu;\alpha\beta}$ is a linear combination of the components of $\partial_\mu T_{\mu\nu}$ with field-independent coefficients . All WIs associated with 4-dimensional rotations can thus be derived from those discussed in the previous section. It is, however, instructive to consider properly chosen integrated WIs. They can be obtained by integrating over a bounded region R which contains in its interior the points $x^1,\dots,x^m$ while the fields $O_{m+1}\dots O_n$ are localized outside. This leads to

$$w_{\alpha\beta}\int_R d^4x\,\langle \partial_\mu K_{\mu;\alpha\beta}(x)\,O_1\dots O_n\rangle = -2\sum_{i=1}^{m}\,\langle O_1\dots\delta_w O_i\dots O_n\rangle \tag{2.23}$$

where $\delta_w O_i$ is the variation of O_i under the *global* transformations associated with $w_{\alpha\beta}$. In particular it is interesting to consider an infinitesimal boost, that in the Euclidean is obtained by choosing $\omega_{0j} = v_j$ and all other components null, an integration region R which is a thick-time slice between the two hyper-planes with $x_0 = y_0 \pm t$, and a correlation function with a field $\overline{T}_{0k}(y_0)$ inserted inside R while the operators $O_1\dots O_n$ are localized outside. The variation of space-time components of the energy-momentum tensor under a global boost reads

$$\delta T_{0k}(y) = v_j\Big\{y_0\,\partial_j T_{0k}(y) - y_j\,\partial_0 T_{0k}(y) + T_{jk}(y) - \delta_{jk}T_{00}(y)\Big\}\ , \tag{2.24}$$

and the integrated WIs can thus be written as

$$\begin{aligned}&\int_{\partial R} d\sigma_\mu(x)\,\langle K_{\mu;0j}(x)\,T_{0k}(y)\,O_1\dots O_n\rangle = \\ &-\langle\Big\{y_0\partial_j T_{0k}(y) - y_j\partial_0 T_{0k}(y) + T_{jk}(y) - \delta_{jk}T_{00}(y)\Big\}\,O_1\dots O_n\rangle\ .\end{aligned} \tag{2.25}$$

By using Eq. (2.8), and for correlation functions for which boundary terms can be neglected when integrating by parts in d^3y, such as connected correlations functions with operators O_i localized in space, the WIs read

$$\int_{\partial R} d\sigma_\mu(x)\,\langle K_{\mu;0j}(x)\overline{T}_{0k}(y_0)\,O_1\dots O_n\rangle_c = \delta_{jk}\,\langle\overline{T}_{00}(y_0)\,O_1\dots O_n\rangle_c\ . \tag{2.26}$$

Being valid for every string of external localized operators, i.e. for a generic state, this is the Euclidean version of the commutation relation of the momentum with the charges associated with the boosts. Finally it is interesting to notice that the number of fields $T_{\mu\nu}$ inserted in the correlation functions entering the two sides of these WIs is different.

3 Momentum distribution from shifted boundaries

In this section we show how the correlation functions of the total momentum can be extracted in the Euclidean path integral formalism by generalizing the periodic temporal boundary condition to shifted boundary conditions. The relative contribution to the partition function of the states with momentum $\mathbf{p}$ is (L_0 dependence suppressed)

$$\frac{R(\mathbf{p})}{V} = \frac{\mathrm{Tr}\{e^{-L_0\hat{\mathrm{H}}}\,\hat{\mathrm{P}}^{(\mathbf{p})}\}}{\mathrm{Tr}\{e^{-L_0\hat{\mathrm{H}}}\}}\;, \tag{3.1}$$

where the trace is over all the states of the Hilbert space, $\hat{\mathrm{P}}^{(\mathbf{p})}$ is the projector onto those states with total momentum $\mathbf{p}$, and $\hat{\mathrm{H}}$ is the Hamiltonian of the theory. If we introduce the partition function

$$Z(\mathbf{z}) = \mathrm{Tr}\{e^{-L_0\hat{\mathrm{H}}}\,e^{i\hat{\mathbf{p}}\mathbf{z}}\}\;, \tag{3.2}$$

in which states of momentum $\mathbf{p}$ are weighted by a phase $e^{i\mathbf{p}\cdot\mathbf{z}}$, and we use the standard group theory machinery (see Ref. [12] for a detailed discussion on this point) it easy to show that

$$R(\mathbf{p}) = \frac{1}{Z}\int d^3\mathbf{z}\,e^{-i\mathbf{p}\cdot\mathbf{z}}\,Z(\mathbf{z})\;, \tag{3.3}$$

where $Z = Z(\mathbf{0})$ is the ordinary thermal partition function. The generating function $K(\mathbf{z})$ of the cumulants of the momentum distribution is defined as usual as

$$e^{-K(\mathbf{z})} = \frac{1}{V}\sum_{\mathbf{p}} e^{i\mathbf{p}\cdot\mathbf{z}}\,R(\mathbf{p})\;, \tag{3.4}$$

and the cumulants are given by

$$k^V_{\{2n_1,2n_2,2n_3\}} = (-1)^{n_1+n_2+n_3+1}\,\frac{\partial^{2n_1}}{\partial\mathbf{z}_1^{2n_1}}\frac{\partial^{2n_2}}{\partial\mathbf{z}_2^{2n_2}}\frac{\partial^{2n_3}}{\partial\mathbf{z}_3^{2n_3}}\frac{K(\mathbf{z})}{V}\Big|_{\mathbf{z}=0}\;, \tag{3.5}$$

where they have been normalized so as to have a finite limit when $V\to\infty$. The shifted partition function $Z(\mathbf{z})$ can be expressed as a Euclidean path integral with the field satisfying the boundary conditions

$$\phi(L_0,\mathbf{x}) = \phi(0,\mathbf{x}+\mathbf{z}) \tag{3.6}$$

in the compact direction. From Eqs. (3.3) and (3.4), the generating function can thus be written as the ratio of partition functions

$$e^{-K(\mathbf{z})} = \frac{Z(\mathbf{z})}{Z}\;, \tag{3.7}$$

i.e. two path integrals with the same action but different boundary conditions, and the cumulants can be obtained by deriving it with respect to the shift parameter z an appropriate number of times. Since the cumulants are connected correlation functions of the total momentum charge of the theory, they are ultraviolet finite as they stand (see also section 5 and appendix A). Therefore $K(\mathbf{z})$ and the momentum distribution $R(\mathbf{p})$ are finite as well, and they do not need any ultra-violet renormalization.

3.1 Extension to the lattice

When defined on a lattice, the theory is invariant under a discrete subgroup of translations and rotations only, the momenta are quantized, and the continuum WIs are broken by discretization effects. Generic lattice definitions of the energy-momentum tensor, as well as the corresponding charges, require ultraviolet renormalization. It is still possible, however, to factorize the Hilbert space of the lattice theory in sectors with definite conserved total momentum. The formula for the lattice projector $\hat{\mathrm{P}}^{(\mathbf{p})}$ can be easily obtained, and its explicit form can be found in Ref. [12]. Since only physical states contribute to the symmetry constrained path integrals in Eq. (3.1), the lattice momentum distribution $R(\mathbf{p})$ is expected to converge to the continuum universal one without the need for any ultra-violet renormalization. The definition of the cumulants in Eq. (3.5) is thus applicable at finite lattice spacing, provided the derivatives are replaced with their discrete counterpart, and no additive or multiplicative ultraviolet-divergent renormalization is needed for taking the continuum limit.

4 Two-point correlators of $T_{\mu\mu}$

The two-point correlation functions of the diagonal components of the energy-momentum tensor satisfy WIs which are non-trivial and interesting in the thermal theory at finite volume. By choosing $T_{kk}(y)$ as interpolating operator, $\epsilon_\nu = \delta_{\nu 0}\epsilon_0$ and by using translational invariance and parity, the WI (2.6) can be written as

$$\partial_0^x \Big\{ \langle \overline{T}_{00}(x_0)\, T_{kk}(y)\rangle + \delta(x_0 - y_0)\, \langle T_{00} + \mathcal{L}\rangle \Big\} = 0 \, . \tag{4.1}$$

Analogously by taking $\epsilon_\nu = \delta_{\nu k}\epsilon_k$, $T_{00}(z)$ as interpolating operator, and by using translational invariance and "k-parity"

$$\partial_k^w \Big\{ \langle \widetilde{T}_{kk}(w_k)\, T_{00}(z)\rangle + \delta(w_k - z_k)\, \langle T_{kk} + \mathcal{L}\rangle \Big\} = 0 \, , \tag{4.2}$$

where

$$\widetilde{T}_{\mu\nu}(w_k) = \int \Big[\prod_{\rho \neq k} dw_\rho \Big]\, T_{\mu\nu}(w) \, . \tag{4.3}$$

By integrating both of them and by taking the difference, we obtain ($x_0 \neq y_0 \, , w_k \neq z_k$)

$$L_0\, \langle \overline{T}_{00}(x_0)\, T_{kk}(y)\rangle - L_k\, \langle \widetilde{T}_{kk}(w_k)\, T_{00}(z)\rangle = \langle T_{00}\rangle - \langle T_{kk}\rangle \, . \tag{4.4}$$

If we subtract from both terms on the l.h.s the disconnected piece, we arrive at

$$L_0\, \langle \overline{T}_{00}(x_0)\, T_{kk}(y)\rangle_c - L_k\, \langle \widetilde{T}_{kk}(w_k)\, T_{00}(z)\rangle_c = \langle T_{00}\rangle - \langle T_{kk}\rangle \, . \tag{4.5}$$

Non-trivial properties of Eqs. (4.4)-(4.5) are that all operators are localized at non-zero physical distance from each other, that the number of fields $T_{\mu\mu}$ inserted in the correlation functions entering the two sides of each equation is different, and that the

additive renormalization counter-terms proportional to a_1 and a_2 in Eq. (A.3) do not contribute. These equations are thus valid for the renormalized energy-momentum tensor as well, or conversely they imply that the overall renormalization constant satisfies $\mathcal{Z} = 1$ (see appendix A). In regularizations that break translational invariance, they can be imposed to compute non-perturbatively the overall renormalization constant of the diagonal component of the field $T_{\mu\nu}$.

4.1 Thermodynamic limit and finite-size effects

In the thermodynamic limit the second term on the l.h.s. of Eq. (4.5) vanishes, and the infinite volume WI reads

$$L_0 \langle \overline{T}_{00}(x_0)\, T_{kk}(y)\rangle_c = \langle T_{00}\rangle - \langle T_{kk}\rangle \; . \tag{4.6}$$

The very same WI can be obtained in a slightly more elegant form. By integrating a combination of two of the WIs in Eq. (2.6), and by using translational invariance and parities we obtain

$$\int d^4x\, \langle x_0\, \partial_\mu T_{\mu 0}(x)\, T_{kk}(y) - x_k\, \partial_\mu T_{\mu k}(x)\, T_{00}(z)\rangle = \langle T_{00}\rangle - \langle T_{kk}\rangle \; , \tag{4.7}$$

from which it is easy to derive Eq. (4.6). The latter has a straightforward thermodynamic interpretation. If we remember that in the Euclidean

$$\langle T_{00}\rangle = -e \; , \qquad \langle T_{kk}\rangle = p \; , \tag{4.8}$$

where e and p are the energy density and the pressure in the thermodynamic limit respectively, Eqs. (2.14) and (4.6) imply the well-known thermodynamic relation

$$T\frac{\partial p}{\partial T} = e + p \; . \tag{4.9}$$

By defining the entropy density of the finite-volume system as usual

$$s^V = \frac{1}{V}\frac{\partial}{\partial T}\Big[T \ln Z\Big] \; , \tag{4.10}$$

and by using Eq. (2.14) and the analogous one in the k-direction (see Eq. B.4)), the extensivity of the free energy and Eq. (4.9) lead to

$$Ts = e + p \qquad \Longrightarrow \qquad \frac{\partial}{\partial T}\, p = s \; . \tag{4.11}$$

The leading finite-size corrections in these thermodynamic potentials were calculated in Ref. [15] for a generic theory with a mass gap M in the screening spectrum. For the sum of the energy and pressure they read

$$\langle T_{kk}\rangle - \langle T_{00}\rangle - (e + p) = -\frac{\nu M T}{2\pi L}\Big[M + 3T\frac{\partial M}{\partial T}\Big] e^{-ML} + \dots \; , \tag{4.12}$$

where the factor ν stands for the multiplicity of the lightest screening state, and the dots stand for terms which vanish with a larger exponent. The WI (4.5) generalizes Eq. (4.9) to finite-volume, and it shows that the violations in the latter are due to the finite-volume dependence of the energy density, i.e.

$$\langle T_{kk}\rangle - \langle T_{00}\rangle - T\frac{\partial\langle T_{kk}\rangle}{\partial T} = L_k \frac{\partial\langle T_{00}\rangle}{\partial L_k}\ . \tag{4.13}$$

By inserting the finite-size corrections computed in Ref. [15] we obtain

$$T\,\frac{\partial\langle T_{kk}\rangle}{\partial T} - \langle T_{kk}\rangle + \langle T_{00}\rangle = \frac{\nu M^2 T^2}{2\pi}\left(\frac{\partial M}{\partial T}\right)\left[1+\frac{1}{ML}\right]e^{-ML} + \dots\ , \tag{4.14}$$

and analogously for the violation of first equation (4.11)

$$Ts^V - \langle T_{kk}\rangle + \langle T_{00}\rangle = \frac{\nu T}{2\pi L^3}\Big[3+3ML+M^2L^2\Big]e^{-ML} + \dots \tag{4.15}$$

Finite-volume effects in the thermodynamic relations (4.9) and (4.11) are exponentially small in ML, and the leading finite-size corrections are known functions of the lightest screening mass, its temperature derivative and the multiplicity of the associated state.

5 Two-point correlators of T_{0k}

In a finite box a generic boost transformation rotates periodic fields to non-periodic ones. Those transformations are incompatible with the boundary conditions of the finite-volume theory. The integrated WIs associated with the $SO(4)$ rotations must be modified by finite-size contributions which vanishes in the thermodynamic limit. On the other hand the finite-volume theory has an energy-momentum tensor which is locally conserved, and the integrated WIs associated with a generic infinitesimal rotation $\omega_{\alpha\beta}$ can be constructed starting from Eqs. (2.6) and by multiplying both sides by the proper factors. By choosing $\epsilon_\nu = \delta_{\nu k}\epsilon_k$, $T_{0k}(y)$ as interpolating operator, and by using translational invariance and parity, the WI (2.6) can be written as

$$\partial_0^x\Big\{\langle \overline{T}_{0k}(x_0)\,T_{0k}(y)\rangle - \delta(x_0-y_0)\,\langle T_{kk}+\mathcal{L}\rangle\Big\} = 0\ . \tag{5.1}$$

Analogously by taking $\epsilon_\nu = \delta_{\nu 0}\epsilon_0$, $T_{0k}(z)$ as interpolating operator, and by using translational invariance and parity

$$\partial_k^w\Big\{\langle \widetilde{T}_{0k}(w_k)\,T_{0k}(z)\rangle - \delta(w_k-z_k)\,\langle T_{00}+\mathcal{L}\rangle\Big\} = 0\ . \tag{5.2}$$

By integrating both of them and by taking the difference we obtain[4] ($x_0 \neq y_0\ , w_k \neq z_k$)

$$L_0\,\langle \overline{T}_{0k}(x_0)\,T_{0k}(y)\rangle - L_k\langle \widetilde{T}_{0k}(w_k)\,T_{0k}(z)\rangle = \langle T_{00}\rangle - \langle T_{kk}\rangle\ . \tag{5.3}$$

[4]This relation is explicitly verified for the free theory in appendix C.

This WI can be derived directly from Eq. (2.25) by paying attention to the fact that boundary terms in the integration by parts cannot be neglected. The comments below Eq. (4.6) apply also in this case. In particular, in regularizations that break translational invariance, these equations can be imposed to compute non-perturbatively the overall renormalization constant of the off-diagonal components of the field $T_{\mu\nu}$. These WIs are reminiscent of those associated with non-singlet chiral symmetry in QCD, which turn out to be so relevant to renormalize the axial current when chiral symmetry is explicitly broken by the regularization [16, 17] (see also Ref. [18] for a review). From Eqs. (4.5) and (5.3) we obtain

$$\langle \overline{T}_{0k}(x_0) T_{0k}(y)\rangle - \langle \overline{T}_{00}(x_0') T_{kk}(y')\rangle_c = \frac{L_k}{L_0}\Big\{\langle \widetilde{T}_{0k}(w_k) T_{0k}(z)\rangle - \langle \widetilde{T}_{kk}(w_k') T_{00}(z')\rangle_c\Big\}\,, \tag{5.4}$$

where in all correlators the operators must be inserted at a physical distance ($x_0 \neq y_0$, etc.). It is interesting to notice that this relation can be derived directly from the conservation of the energy-momentum tensor in Eq. (2.8) without explicit reference to the transformation properties of the interpolating operators, see Ref. [9] and below.

5.1 Thermodynamic limit and finite-size effects

In the infinite-volume limit the second term on the l.h.s. of Eq. (5.3) vanishes, and the relation reads

$$L_0\, \langle \overline{T}_{0k}(x_0)\, T_{0k}(y)\rangle = \langle T_{00}\rangle - \langle T_{kk}\rangle\ . \tag{5.5}$$

Its thermodynamic interpretation is straightforward. If we remember that in the Euclidean the momentum operator maps to $\hat{p}_k \to -i\overline{T}_{0k}$, then ($x_0 \neq y_0$)

$$\langle \overline{T}_{03}(x_0)\, T_{03}(y)\rangle = -k_{\{0,0,2\}}\ . \tag{5.6}$$

The Eq. (5.5) can then be written as

$$k_{\{0,0,2\}} = T(e+p) = T^2 s\ . \tag{5.7}$$

The WI (5.3) generalizes this equation to finite-volume. The second term on the left-hand side of (5.3) vanishes exponentially in the lowest screening level corresponding to a state with a non-zero momentum in the time direction. Whenever the lightest screening state has vanishing momentum in the time direction, which is expected to be the (generic) case, the leading finite-volume corrections to the second cumulant are those from the r.h.s. of the Eq. (5.3). They are exponentially small in ML, and their explicit form is given by the r.h.s. of Eq. (4.12) multiplied by T.

6 Recursion relation for $2n$-point correlators of $\overline{T}_{0k}$

In the thermodynamic limit the WIs (2.6) imply a recursion relation among correlators of $\overline{T}_{0k}$ inserted at a physical distance. It can be derived by repeatedly using Eq. (2.6) with

different strings of interpolating operators. This can be concisely shown by introducing a new action

$$S_J = S - \int d^4x \, J(x_0) \, T_{0k}(x) \tag{6.1}$$

which differs from the standard one by a term which couples an external source $J(x_0)$, constant over the time-slices, with the momentum field in direction k. The corresponding path-integral is defined as

$$Z[J] = \int D\phi \; e^{-S_J} \; , \tag{6.2}$$

and the expectation value of a generic operator $\langle O \rangle_J$ is defined as usual. It turns out to be useful to introduce the operators $\mathcal{D}_{[x_0^1..x_0^n]}$ defined as

$$\mathcal{D}_{[x_0^1..x_0^n]} \, F(J) = \frac{\partial}{\partial J(x_0^n)} \cdots \frac{\partial}{\partial J(x_0^1)} \, F(J) \Big|_{J=0} \; , \tag{6.3}$$

where $F(J)$ is a generic functional of the external source and the x_0^i are all different. As usual when applied to $F(J) = \ln Z[J]$ it gives the *connected* correlation functions of n momentum operators $\overline{T}_{0k}(x_0^i)$ inserted at a physical distance. By choosing $\epsilon_\nu = \delta_{\nu k} \epsilon_k$ (no summation over k), $\tilde{\tilde{\overline{T}}}_{00}$ as interpolating operator, where

$$\tilde{\tilde{\overline{T}}}_{\mu\nu}(x) = \int \Big[\prod_{\rho \neq 0,k} dx_\rho \Big] \, T_{\mu\nu}(x) \; , \tag{6.4}$$

and by using translational invariance in time[5], the WI (2.6) gives

$$\partial_0^{x^1} D_{[x_0^3..x_0^{2n}]} \langle \tilde{\tilde{\overline{T}}}_{00}(x^1) \, \tilde{\tilde{\overline{T}}}_{0k}(x^2) \rangle_{J,c} = \partial_k^{x^2} D_{[x_0^3..x_0^{2n}]} \langle \tilde{\tilde{\overline{T}}}_{kk}(x^2) \, \tilde{\tilde{\overline{T}}}_{00}(x^1) \rangle_{J,c} \; . \tag{6.5}$$

Analogously by taking $\epsilon_\nu = \delta_{\nu 0} \epsilon_0$, $\tilde{\tilde{\overline{T}}}_{0k}$ as interpolating operator, and thanks to translational invariance and the symmetry of T_{0k}, the WI (2.6) leads also to

$$\partial_0^{x^1} D_{[x_0^3..x_0^{2n}]} \langle \tilde{\tilde{\overline{T}}}_{00}(x^1) \, \tilde{\tilde{\overline{T}}}_{0k}(x^2) \rangle_{J,c} = \partial_k^{x^2} D_{[x_0^3..x_0^{2n}]} \langle \tilde{\tilde{\overline{T}}}_{0k}(x^1) \, \tilde{\tilde{\overline{T}}}_{0k}(x^2) \rangle_{J,c} \; . \tag{6.6}$$

By putting together last two WIs we arrive at

$$\partial_k^{x^2} D_{[x_0^3..x_0^{2n}]} \Big\{ \langle \tilde{\tilde{\overline{T}}}_{0k}(x^2) \, \tilde{\tilde{\overline{T}}}_{0k}(x^1) \rangle_{J,c} - \langle \tilde{\tilde{\overline{T}}}_{kk}(x^2) \, \tilde{\tilde{\overline{T}}}_{00}(x^1) \rangle_{J,c} \Big\} = 0 \; . \tag{6.7}$$

Since the argument of the partial derivative is constant in x_k^2, we can integrate by keeping all insertions at a physical distance (x_0^i all different) and obtain

$$\begin{aligned} & D_{[x_0^3..x_0^{2n}]} \Big\{ \langle \overline{T}_{0k}(x_0^1) \, \overline{T}_{0k}(x_0^2) \rangle_{J,c} - \langle \overline{T}_{00}(x_0^1) \, \overline{T}_{kk}(x_0^2) \rangle_{J,c} \Big\} = \\ & L_k^2 \; D_{[x_0^3..x_0^{2n}]} \Big\{ \langle \tilde{\tilde{\overline{T}}}_{0k}(x^1) \, \tilde{\tilde{\overline{T}}}_{0k}(x^2) \rangle_{J,c} - \langle \tilde{\tilde{\overline{T}}}_{00}(x^1) \tilde{\tilde{\overline{T}}}_{kk}(x^2) \, \rangle_{J,c} \Big\} \; , \end{aligned} \tag{6.8}$$

[5] When an operator $D_{[x_0^1..x_0^{2n}]}$ is applied, the action entering the definition of the correlation functions is the standard one.

which generalizes Eq (5.4). The Eqs. (B.5) and (B.11) give

$$\mathcal{D}_{[x_0^3..x_0^{2n}]} \Big\{ L_0 \,\langle \overline{T}_{kk}(x_0^2) \rangle_J - L_k \,\frac{\partial}{\partial L_k} \ln Z[J] \; - \int dw_0 \; J(w_0) \,\langle \overline{T}_{0k}(w_0) \rangle_J \; , \Big\} = 0 \qquad (6.9)$$

where again the x_0^i are all different, and (a generalization of) Eq. (2.14) leads to

$$D_{[x_0^3..x_0^{2n}]} \langle \overline{T}_{00}(x_0^1) \, \overline{T}_{kk}(x_0^2) \rangle_{J,c} = \frac{\partial}{\partial L_0} \; D_{[x_0^3..x_0^{2n}]} \langle \overline{T}_{kk}(x_0^2) \rangle_J \; . \qquad (6.10)$$

Finally, by putting together the last three equations, we can write (all insertions at a physical distance from each other)

$$\begin{aligned} \langle \overline{T}_{0k}(x_0^1) \ldots \overline{T}_{0k}(x_0^{2n}) \rangle_c &= (2n-1) \, \frac{\partial}{\partial L_0} \, \Big\{ \frac{1}{L_0} \, \langle \overline{T}_{0k}(x_0^3) \ldots \overline{T}_{0k}(x_0^{2n}) \rangle_c \Big\} \, + \\ L_k^2 \Big\{ \langle \widetilde{\overline{T}}_{0k}(x^1) \, \widetilde{\overline{T}}_{0k}(x^2) \overline{T}_{0k}(x_0^3) \ldots \overline{T}_{0k}(x_0^{2n}) \rangle_c &- \langle \widetilde{\overline{T}}_{00}(x^1) \, \widetilde{\overline{T}}_{kk}(x^2) \, \overline{T}_{0k}(x_0^3) \ldots \overline{T}_{0k}(x_0^{2n}) \rangle_c \Big\} \\ + \frac{\partial}{\partial L_0} \Big\{ \frac{1}{L_0} \Big[L_k \frac{\partial}{\partial L_k} - 1 \Big] \langle \overline{T}_{0k}(x_0^3) \ldots \overline{T}_{0k}(x_0^{2n}) \rangle_c \Big\} \; . & \qquad (6.11) \end{aligned}$$

6.1 Thermodynamic limit and finite-size effects

The last three terms in Eq. (6.11) are finite-size effects which vanish in the infinite volume limit: the first two because the distance $|x_k^1 - x_k^2|$ can be arbitrarily large, the third one due to the expected volume dependence of the correlation function. In the thermodynamic limit we thus arrive at the recursive relation

$$\langle \overline{T}_{0k}(x_0^1) \ldots \overline{T}_{0k}(x_0^{2n}) \rangle_c = (2n-1) \, \frac{\partial}{\partial L_0} \, \Big\{ \frac{1}{L_0} \, \langle \overline{T}_{0k}(x_0^3) \ldots \overline{T}_{0k}(x_0^{2n}) \rangle_c \Big\} \; , \qquad (6.12)$$

with a straightforward thermodynamic interpretation

$$k_{\{0,0,2n\}} = (2n-1) T^2 \frac{\partial}{\partial T} \Big\{ T \, k_{\{0,0,2n-2\}} \Big\} \; . \qquad (6.13)$$

Cumulants with non-trivial indices in the other two spatial directions are related to those in Eq. (6.13) by cubic symmetry. For the total momentum, Eq. (6.12) is the analog of the well-known recursive relation among the connected correlation functions of the energy, see Eq. (2.14) with $\mathcal{O}$ being a string of $\overline{T}_{00}$'s. The Eq. (6.13) is checked explicitly in appendix D for the free theory. It is interesting to notice that it leads to a straightforward physical interpretation of the fourth cumulant, i.e.

$$k_{\{0,0,4\}} = 3T^4 c_v + 9T^3 (e+p) \; , \qquad (6.14)$$

where c_v is the specific heat of the system in the thermodynamic limit. Finite-volume corrections to this identity can be computed by starting from the WIs (B.1) and by

following a procedure analogous to the one which lead to Eq. (5.3). For the fourth cumulant the relevant WI reads[6]

$$L_0^3 \langle \overline{T}_{0k}\overline{T}_{0k}\overline{T}_{0k}T_{0k}\rangle_c - L_k^3 \langle \widetilde{T}_{0k}\widetilde{T}_{0k}\widetilde{T}_{0k}T_{0k}\rangle_c = 3\Big\{\langle T_{00}\rangle - \langle T_{kk}\rangle\Big\} \tag{6.15}$$

$$-3\Big\{L_0 \langle \overline{T}_{00}T_{00}\rangle_c - L_k \langle \widetilde{T}_{kk}T_{kk}\rangle_c\Big\} + 6\Big\{L_0^2 \langle \overline{T}_{0k}\overline{T}_{0k}T_{00}\rangle_c - L_k^2 \langle \widetilde{T}_{0k}\widetilde{T}_{0k}T_{kk}\rangle_c\Big\}\ .$$

To compute the leading finite-size effects, it is convenient to rewrite this equation as

$$L_0^3 \langle \overline{T}_{0k}\overline{T}_{0k}\overline{T}_{0k}T_{0k}\rangle_c = 3\Big\{L_0\frac{\partial}{\partial L_0} - L_k\frac{\partial}{\partial L_k} - 2\Big\}\Big\{\langle T_{00}\rangle - \langle T_{kk}\rangle\Big\}$$

$$+L_k^3 \langle \widetilde{T}_{0k}\widetilde{T}_{0k}\widetilde{T}_{0k}T_{0k}\rangle_c - 6L_k\Big\{1 + L_k\frac{\partial}{\partial L_k} - L_0\frac{\partial}{\partial L_0}\Big\}\langle \widetilde{T}_{0k}T_{0k}\rangle\ . \tag{6.16}$$

The second line of the right-hand side vanishes exponentially in the lowest screening level corresponding to a state with non-zero momentum in the time direction. We therefore turn our attention to the first line, from which we compute the leading finite-size corrections to the fourth cumulant by using again the results in Ref. [15]

$$T^{-3} \langle \overline{T}_{0k}\overline{T}_{0k}\overline{T}_{0k}T_{0k}\rangle_c - 3Tc_v - 9(e+p) = -\frac{3\nu T}{2\pi L}\Big\{3\,\frac{\partial}{\partial T}\Big(e^{-ML}MT^2\,\tfrac{\partial M}{\partial T}\Big) +$$

$$e^{-ML}\,MT\,\frac{\partial M}{\partial T}\,(7-2ML) - \frac{e^{-ML}}{L^2}\,(6+6ML+M^3L^3)\Big\} + \dots \tag{6.17}$$

where the dots stand for terms that vanish exponentially faster.

7 Main results and conclusions

By comparing the WI (5.7) and the Eq. (3.5) with $n_3 = 1$ and $n_1 = n_2 = 0$, the entropy density in the thermodynamic limit can be written as

$$s = -\frac{1}{T^2}\lim_{V\to\infty}\frac{1}{V}\frac{d^2}{dz^2}\ln Z(\{0,0,z\})\Big|_{z=0}\ . \tag{7.1}$$

Thanks to Eq. (4.11), the pressure can be computed by integrating s in the temperature, and the ambiguity left due to the integration constant is consistent with the fact that p is defined up to an arbitrary additive renormalization constant. From the relation (6.14), the specific heat of the system can be written as

$$c_v = \lim_{V\to\infty}\frac{1}{V}\left[\frac{1}{3T^4}\frac{d^4}{dz^4} + \frac{3}{T^2}\frac{d^2}{dz^2}\right]\ln Z(\{0,0,z\})\Big|_{z=0}\ . \tag{7.2}$$

The last two equations make clear that the response of the partition function to the shift z is governed by basic thermodynamic properties of the system, and that the potentials

[6] In this and next equation the arguments x_0^i and x_k^i are omitted. Operators are inserted always at a physical distance.

entering the equation of state of the thermal theory can be extracted by rather simple formulas. It is worth stressing that Eqs. (7.1) and (7.2) are the result of a judicious combination of the WIs associated with invariance of the theory under the Poincaré group only. The relevant WIs relate correlation functions of conserved charges, and this is why they are free from ultraviolet subtractions and renormalizations. The formulas (7.1) and (7.2) are indeed valid for a wider class of thermal field theories than the scalar one [9]. For gauge theories, however, their derivation involves additional complications due to the non-commutation of translations and gauge transformations, and it will be presented in a forthcoming paper [10].

Crucially the Eqs. (7.1) and (7.2) remain valid in a lattice box, up to exponentially suppressed finite-size effects and harmless discretization errors, provided the derivatives are replaced with their discrete counterpart. In a finite volume some of the relevant WIs generalize well-known thermodynamic relations, and they are the basic ingredient to relate the finite-size effects in the cumulants to those in simple quantities such as the energy density and pressure which are known [15]. With respect to the analogous observables computed in the standard methods [5–8], the entropy density and the specific heat computed from the equations above do require neither a vacuum subtraction nor an ultraviolet renormalization constant to be fixed. Moreover an improvement of the action automatically leads to a corresponding improvement in the thermodynamic quantities. Conversely the shifted boundary conditions adopted in this paper and the WIs (4.5) and (5.3), which are valid for the renormalized energy-momentum tensor as well, can be combined to design a non-perturbative renormalization procedure for $T_{\mu\nu}$ on the lattice.

The generating function $K(\mathbf{z})$ may turn out to be an interesting thermodynamic quantity in itself. For a scale-invariant theory, for instance, one might have expected that $K(\mathbf{z})$ can be an arbitrary function of $T|\mathbf{z}|$. However, the recurrence relation (6.13) and the scale invariance fix its functional form unambiguously to be

$$\frac{K(\mathbf{z})}{V} = \frac{s}{4}\left[1 - \frac{1}{(1+T^2\mathbf{z}^2)^2}\right] , \tag{7.3}$$

no matter what the coupling of the theory is. This is particularly relevant to those strongly coupled theories that can be treated with the AdS/CFT correspondence. We note that for $\mathbf{z}$ purely imaginary, $\mathbf{v} \equiv iT\mathbf{z}$ can be interpreted as the macroscopic velocity of the thermal system. The double poles in $\mathbf{z}$ appearing in Eq. (7.3) corresponding to $|\mathbf{v}| = 1$ therefore do not come as a surprise.

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A Renormalization pattern of $T_{\mu\nu}$

The renormalization pattern of the energy-momentum tensor was studied in great detail in perturbation theory [19–23]. Here we assume to work in a regularization which preserves translational invariance, such as the dimensional one [19–22]. A more general analysis, which is needed for the lattice theory can be found in [23]. Since the ϕ^4 theory is not asymptotically free, it is difficult to extend the results reviewed here non-perturbatively. For the scope of this appendix, however, the standard power counting argument is sufficient.

The bare energy-momentum tensor is a dimension-4 field, symmetric under the exchange $\mu \leftrightarrow \nu$, even under the transformation $\phi \to -\phi$, and which satisfies the conservation equation (2.8). The renormalized tensor can thus be written as

$$\widehat{T}_{\mu\nu} = \mathcal{Z}\left\{T_{\mu\nu} + a_1\left[\delta_{\mu\nu}\Box - \partial_\mu\partial_\nu\right]\phi^2 + a_2\,\delta_{\mu\nu}\right\}\ . \tag{A.1}$$

Since by construction the last two fields on the r.h.s. have zero divergence, $\widehat{T}_{\mu\nu}$ satisfies the conservation equations (2.8) as well. If we choose the O_i to be a combination of elementary fields, the integrated WIs (2.9) can be written as

$$\frac{\epsilon_\nu}{\mathcal{Z}}\int_{\partial R} d\sigma_\mu(x)\,\langle \widehat{T}_{\mu\nu}(x)\widehat{O}_1\ldots\widehat{O}_n\rangle = -\sum_{i=1}^{n}\left\langle \widehat{O}_1\ldots\delta_\epsilon\widehat{O}_i\ldots\widehat{O}_n\right\rangle\ , \tag{A.2}$$

where $\widehat{O}_i$ are the corresponding renormalized fields, and the contributions proportional to a_1 and a_2 vanish because they are surface integrals of vectors with null divergence. Since the correlation functions entering Eq. (A.2) are finite by construction, then also $\mathcal{Z}$ must be finite. If we choose $\mathcal{Z}=1$, the renormalized energy-momentum tensor reads

$$\widehat{T}_{\mu\nu} = T_{\mu\nu} + a_1\left[\delta_{\mu\nu}\Box - \partial_\mu\partial_\nu\right]\phi^2 + a_2\,\delta_{\mu\nu} \tag{A.3}$$

and it satisfies WIs of the same form as those of the bare field, i.e. Eqs. (2.8) and (2.9). The last two fields on the r.h.s. of Eq. (A.3) do not contribute to the charges $\overline{T}_{0k}(x_0)$, since the integration by parts of the term proportional to a_1 gives no boundary contributions. The physical momentum fields are therefore defined by their bare expressions, and no renormalization ambiguity is left. The field proportional to a_2 contributes to the charge $\overline{T}_{00}(x_0)$ by an additive constant term a_2L^3, which is ultraviolet divergent and proportional to the volume of the system. It contributes to the vacuum expectation value of the energy, but it cancels in connected correlation functions of $\overline{T}_{00}$ with other fields. An analogous analysis applies for the fields $\widetilde{T}_{k\nu}(x_k)$ ($\nu \neq k$) and $\widetilde{T}_{kk}(x_k)$. They are the momenta and the energy if direction k is interpreted as the "time" direction. In particular the divergent coefficient a_2 is the very same for $\overline{T}_{00}(x_0)$ and $\widetilde{T}_{kk}(x_k)$.

The second term on the r.h.s. of Eq. (A.3) (as well as the third one) contributes to the trace $T_{\mu\mu}$ of the energy momentum-tensor. In the quantum theory the renormalization procedure indeed breaks the conformal invariance of the classical theory also in the massless limit (trace anomaly).

B Ward identities in presence of external sources

In this appendix we generalize some of the results of section 2 to the theory defined by the action S_J given in Eq. (6.1). The starting point are the the WIs

$$\epsilon_\nu \langle \Big\{ \partial_\mu T_{\mu\nu}(x) + J(x_0)\partial_\nu T_{0k}(x) - \partial_0 \left[J(x_0)(T_{\nu k}(x) + \delta_{\nu k}\mathcal{L}(x)) \right] \tag{B.1}$$
$$- J(x_0)\partial_k [T_{\nu 0}(x) + \delta_{\nu 0}\mathcal{L}(x)] \Big\} O_1 \ldots O_n \rangle_J = - \sum_{i=1}^{n} \langle O_1 \ldots \delta_\epsilon^x O_i \ldots O_n \rangle_J \ ,$$

which extend those in Eq. (2.6).

B.1 Evolution and translational invariance in k-direction

From the previous WIs we can derive the "k-time" evolution of a generic field. If we choose $\epsilon_\nu = \delta_{\nu k}\epsilon_k$ (no summation over k) in Eq. (B.1), and we integrate over a thick k-slice R with the field O_1 being inserted into it while the operators $O_2 \ldots O_n$ are localized outside, we obtain

$$\partial_k \langle O_1(x^1)\, O_2 \ldots O_n \rangle_J = - \int_{\partial R} d\sigma_k(x) \, \langle T_{kk}(x)\, O_1(x^1)\, O_2 \ldots O_n \ \rangle_J \ . \tag{B.2}$$

This is the Euclidean version of the k-time evolution of the generic field $O_1(x^1)$, and therefore the field $\widetilde{T}_{kk}$ is the Hamiltonian of the system associated with the k-time. If R covers the full space, we obtain

$$\sum_{i=1}^{n} \partial_k^{x^i} \left\langle O_1(x^1) \ldots O_i(x^i) \ldots O_n(x^n) \right\rangle_J = 0 \ , \tag{B.3}$$

i.e. a generic correlation function is translational invariant in the k direction even in presence of the external source. This is expected since the source field is constant in x_k, and it does not break translational invariance in this direction. By following an analogous procedure, it is straightforward to show that translational invariance is preserved in the other two spatial directions too. Since the field $\widetilde{T}_{kk}$ is the Hamiltonian in direction k, we can write

$$\langle \widetilde{T}_{kk}(x_k) \rangle_J = \frac{\partial}{\partial L_k} \ln Z[J] \ , \tag{B.4}$$

and the independence of the r.h.s from x_k (translational invariance) implies

$$\int d^4x \, \langle T_{kk}(x) \rangle_J = L_k \frac{\partial}{\partial L_k} \ln Z[J] \ . \tag{B.5}$$

B.2 Translational invariance in 0-direction

If we consider Eq. (B.1) for the interpolating field $\overline{T}_{kk}(y_0)$, we choose (no summation over k) $\epsilon_\nu = \epsilon_k \delta_{\nu k}$, and we integrate over the time-slices we obtain

$$\begin{aligned} \partial_0^x \, \langle \overline{T}_{0k}(x_0)\, \overline{T}_{kk}(y_0)\rangle_J &= \partial_0^x \Big\{ J(x_0) \, \langle \Big[\overline{T}_{kk}(x_0) + \overline{\mathcal{L}}(x_0) \Big] \, \overline{T}_{kk}(y_0)\rangle_J \Big\} \\ &+ \Big[\partial_0^y \delta(y_0 - x_0) \Big] \langle \overline{T}_{0k}(y_0)\rangle_J \; . \end{aligned} \tag{B.6}$$

By taking again Eq. (B.1) for the field $\overline{T}_{kk}(y_0)$ but for $\epsilon_\nu = \epsilon_0 \delta_{\nu 0}$, and by integrating over the full space we arrive at

$$\partial_0^y \, \langle \overline{T}_{kk}(y_0)\rangle_J = - \int dx_0 \, J(x_0) \, \partial_0^x \langle \overline{T}_{0k}(x_0)\, \overline{T}_{kk}(y_0)\rangle_J \; . \tag{B.7}$$

If we now put together Eqs. (B.6) and (B.7) we obtain

$$\begin{aligned} \partial_0^y \, \langle \overline{T}_{kk}(y_0)\rangle_J &= - \int dx_0 \, J(x_0) \, \partial_0^x \Big[J(x_0) \langle (\overline{T}_{kk}(x_0) + \overline{\mathcal{L}}(x_0)) \overline{T}_{kk}(y_0)\rangle_J \Big] \\ &- \Big[\partial_0^y J(y_0) \Big] \langle \overline{T}_{0k}(y_0)\rangle_J \; . \end{aligned} \tag{B.8}$$

We are interested in applying the operator $\mathcal{D}_{[x_0^1..x_0^{2n}]}$ defined in Eq. (6.3) on both sides of the last equation. Since the x_0^i are all different from each other, the first term on the r.h.s. of Eq. (B.8) does not contribute, and we obtain

$$\mathcal{D}_{[x_0^1..x_0^{2n}]} \Big\{ \partial_0^y \, \langle \overline{T}_{kk}(y_0)\rangle_J + [\partial_0^y J(y_0)] \, \langle \overline{T}_{0k}(y_0)\rangle_J \Big\} = 0 \; , \tag{B.9}$$

where at most one of the x_0^i can coincides with y_0. In this case

$$\mathcal{D}_{[x_0^1..x_0^{2n}]} \Big\{ J(y_0) \partial_0^y \langle \overline{T}_{0k}(y_0)\rangle_J \Big\} = 0 \tag{B.10}$$

and, since the derivative ∂_0^y commute with $\mathcal{D}_{[x_0^1..x_0^{2n}]}$,

$$\partial_0^y \, \mathcal{D}_{[x_0^1..x_0^{2n}]} \Big\{ \langle \overline{T}_{kk}(y_0)\rangle_J + J(y_0) \, \langle \overline{T}_{0k}(y_0)\rangle_J \Big\} = 0 \; . \tag{B.11}$$

It is reassuring to notice that this equation can be obtained directly from Eq. (2.6) without the need of introducing S_J.

By putting together Eqs. (B.5) and (B.11) we finally obtain Eq. (6.9), i.e.

$$\mathcal{D}_{[x_0^1..x_0^{2n}]} \Big\{ L_0 \, \langle \overline{T}_{kk}(y_0)\rangle_J - L_k \frac{\partial}{\partial L_k} \ln Z[J] \, - \int dw_0 \, J(w_0) \, \langle \overline{T}_{0k}(w_0)\rangle_J \Big\} = 0 \; , \tag{B.12}$$

where y_0 in this equation is different from all x_0^i.

C The Ward Identity (5.3) in the free theory

In this appendix we check explicitly Eq. (5.3) for the free theory. Other WIs, for instance Eqs. (4.5) and (5.4), can be verified analogously. In a finite 4-dimensional volume the propagator

$$\langle\phi(x)\phi(y)\rangle = D(x-y) \tag{C.1}$$

is given by

$$D(x) \equiv \frac{1}{V}\sum_p \frac{e^{ipx}}{p^2+m^2}\ , \tag{C.2}$$

where p runs over a 4-dimensional momentum-space lattice $p_\mu = 2\pi\, n_\mu/L_\mu$ with $\mu = 1,\ldots,4$, and $n_\mu \in \mathcal{Z}$. It satisfies the equation of motion

$$\left\{\Box - m^2\right\} D(x-y) = -\delta^{(\mathrm{p})}(x-y) \tag{C.3}$$

where the periodic function $\delta^{(\mathrm{p})}$ is defined as

$$\delta^{(\mathrm{p})}(x) = \frac{1}{V}\sum_p e^{ipx}\ . \tag{C.4}$$

Thanks to the Wick theorem and to the invariance under parity

$$\begin{aligned}\langle T_{\mu\nu}(x)T_{0k}(y)\rangle = {} & [\partial_\mu\partial_0 D(x-y)]\,[\partial_\nu\partial_k D(x-y)] + [\partial_\mu\partial_k D(x-y)]\,[\partial_\nu\partial_0 D(x-y)]\\ & -\delta_{\mu\nu}\Big\{\,[\partial_\rho\partial_0 D(x-y)]\,[\partial_\rho\partial_k D(x-y)] + m^2\,[\partial_0 D(x-y)]\,[\partial_k D(x-y)]\,\Big\}\ ,\end{aligned} \tag{C.5}$$

where the derivatives are with respect to x. By using the equation of motion (C.3), it is easy to show that

$$\partial_\mu\langle T_{\mu\nu}(x)T_{0k}(y)\rangle = -\Big[\partial_0\delta^{(\mathrm{p})}(x-y)\Big]\,\Big[\partial_\nu\partial_k D(x-y)\Big] - \Big[\partial_k\delta^{(\mathrm{p})}(x-y)\Big]\,\Big[\partial_\nu\partial_0 D(x-y)\Big]\ , \tag{C.6}$$

and by remembering that

$$K_{\mu;0k}(x) = x_0 T_{\mu k}(x) - x_k T_{\mu 0}(x), \tag{C.7}$$

the symmetry of $T_{\mu\nu}$ implies ($y_0 \neq 0$ and $y_k \neq 0$, no summation over k)

$$\int d^4x\,\partial_\mu\langle K_{\mu;0k}(x)T_{0k}(y)\rangle = \partial_k^2 D(z)\Big|_{z=0} - \partial_0^2 D(z)\Big|_{z=0}\ . \tag{C.8}$$

By writing the r.h.s. as

$$\langle T_{00}\rangle - \langle T_{kk}\rangle = \partial_k^2 D(z)\Big|_{z=0} - \partial_0^2 D(z)\Big|_{z=0} \tag{C.9}$$

then Eq. (C.8) corresponds to Eq. (5.3) in the free theory, i.e.

$$\int d^4x\,\partial_\mu\langle K_{\mu;0k}(x)T_{0k}(y)\rangle = \langle T_{00}\rangle - \langle T_{kk}\rangle\ , \qquad y_0 \neq 0\ ,\ \ y_k \neq 0\ . \tag{C.10}$$

D Generating function for free and scale-invariant cases

In this appendix we compute the generating function $K(\mathbf{z})$ of the cumulants of the momentum distribution in the free theory, and check explicitly the recursion relation (6.13). We also compute the same quantity on the lattice to assess the magnitude of discretization effects in realistic computations.

In a finite volume the shifted partition function is given by

$$Z(\mathbf{z}) = \left(\prod_{\mathbf{p}} \sum_{n_{\mathbf{p}}}\right) \exp\left[\sum_{\mathbf{p}} n_{\mathbf{p}} \left(-L_0\, \omega_{\mathbf{p}} + i\mathbf{p}\cdot\mathbf{z}\right)\right] , \tag{D.1}$$

where $\mathbf{p}$ runs over the 3-dimensional momentum-space lattice $\mathbf{p}_i = 2\pi\mathbf{m}_i/L$ with i=1,2,3 and $\mathbf{m}_i \in \mathcal{Z}$. As usual $n_{\mathbf{p}}$ is the occupation number of the single-particle state labeled by $\mathbf{p}$, see Ref. [1]. By performing the geometric sums, the cumulant generator is given by

$$K(\mathbf{z}) = \sum_{\mathbf{p}} \ln \frac{1 - e^{-L_0\omega_{\mathbf{p}} + i\mathbf{p}\cdot\mathbf{z}}}{1 - e^{-L_0\omega_{\mathbf{p}}}} \; . \tag{D.2}$$

In the infinite volume limit

$$\sum_{\mathbf{p}} \to V \int \frac{d^3\mathbf{p}}{(2\pi)^3} \; ,$$

and rotational symmetry is restored. In the massless limit $\omega_{\mathbf{p}} = |\mathbf{p}|$ and, by integrating over the norm of $\mathbf{p}$ first, we obtain

$$\frac{K(\mathbf{z})}{V} = \frac{s}{4}\left[1 - \frac{1}{(1+T^2\mathbf{z}^2)^2}\right] , \tag{D.3}$$

where the entropy density is given by $s = 2\pi^2 T^3/45$. In the massive case $\omega_{\mathbf{p}} = \sqrt{\mathbf{p}^2 + m^2}$, and we proceed by Taylor-expanding the logarithm and by performing the integration over the angular variables

$$\frac{K(\mathbf{z})}{V} = \sum_{n\geq 1} \frac{1}{2\pi^2 n} \int_0^\infty p^2 dp\, e^{-nL_0\omega_{\mathbf{p}}} \left[1 - \frac{\sin(np|\mathbf{z}|)}{np|\mathbf{z}|}\right] . \tag{D.4}$$

By also Taylor-expanding the sinus, and by using the integral representation of the modified Bessel functions $K_\nu(x)$ we obtain

$$\frac{K(\mathbf{z})}{V} = -\frac{m^2 T}{\pi^{5/2}} \sum_{j\geq 1} \frac{1}{j^2} \sum_{n\geq 1} \frac{\Gamma(n+\frac{3}{2})}{(2n+1)!} \left(-2jmT\mathbf{z}^2\right)^n K_{n+2}(jm/T) \, . \tag{D.5}$$

It is straightforward to verify that the cumulants generated from $K(\mathbf{z})$ in Eqs. (D.3) and (D.5) satisfy the recursive relation (6.13). For the massive case, the latter is implied by the recursive relation $\frac{d}{dx}\frac{K_\nu(x)}{x^\nu} = -\frac{K_{\nu+1}(x)}{x^\nu}$ among the modified Bessel functions.

D.1 Free theory on the lattice

Analogously to the continuum, the cumulant generator of the scalar free theory discretized on the hypercubic in the standard way, i.e. with ∂_μ replaced by the forward finite-difference operator, is

$$K(\mathbf{z}) = \sum_{\mathbf{p}} \ln \frac{1 - e^{-L_0\omega_{\mathbf{p}} + i\mathbf{p}\cdot\mathbf{z}}}{1 - e^{-L_0\omega_{\mathbf{p}}}} = \frac{1}{2}\sum_{\mathbf{p}} \ln \frac{\cosh(L_0\,\omega_{\mathbf{p}}) - \cos(\mathbf{p}\cdot\mathbf{z})}{\cosh(L_0\,\omega_{\mathbf{p}}) - 1}\,, \tag{D.6}$$

where

$$a\omega_{\mathbf{p}} = 2\,\mathrm{asinh}\left(\frac{1}{2}a\sqrt{\hat{\mathbf{p}}^2 + m^2}\right)\,, \qquad \hat{\mathbf{p}}^2 = \frac{4}{a^2}\sum_{i=1}^{3}\sin^2\left(\frac{a\,\mathbf{p}_i}{2}\right)\,. \tag{D.7}$$

By expanding in the lattice spacing a, in the thermodynamic limit it is easy to show that discretization effects are well-behaved and scale as expected, i.e. proportionally to $(a/L_0)^2$. In practice one can use $a\omega_{\mathbf{p}} = 2\ln u_{\mathbf{p}}$, $u_{\mathbf{p}} = \frac{1}{2}a\sqrt{\hat{\mathbf{p}}^2 + m^2} + \sqrt{1 + a^2(\hat{\mathbf{p}}^2 + m^2)/4}$, so that $\cosh(L_0\,\omega_{\mathbf{p}}) = \frac{1}{2}(u_{\mathbf{p}}^{2L_0/a} + u_{\mathbf{p}}^{-2L_0/a})$, and carry out the sum over momenta numerically.

D.2 Scale-invariant theories

The functional form in Eq. (D.3) is more generally valid than just for the free massless theory. The combination of scale invariance and of the recursive relation (6.13) fully fixes the cumulant generator $K(\mathbf{z})$. To show this we notice that scale invariance implies

$$k_{\{0,0,2n\}} = c_{\{0,0,2n\}}\,T^{2n+3}\,. \tag{D.8}$$

It is then not difficult to solve the recursion relation (6.13) for $c_{\{0,0,2n\}}$ to find

$$k_{\{0,0,2n\}} = (n+1)\,(2n)!\,\frac{s}{4}\,T^{2n}\,. \tag{D.9}$$

For $\mathbf{z} = \{0,0,z\}$ the cumulant generator can thus be written as

$$K(\{0,0,z\}) = V\sum_{n=1}^{\infty}\frac{(-1)^{n+1}}{(2n)!}\,k_{\{0,0,2n\}}\,z^{2n}\,, \tag{D.10}$$

and by re-summing the series and using rotational invariance Eq. (D.3) is obtained. A priori, one might have expected that in a scale-invariant theory, $K(\mathbf{z})$ can be an arbitrary function of $T|\mathbf{z}|$. However, the Ward identities of energy and momentum conservation fix its functional form unambiguously.

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